MATH AND SCIENCE @ WORK

AP* CHEMISTRY Educator Edition

GENERATING WATER IN SPACE

Instructional Objectives

Students will

- write an equilibrium expression for a reaction;
- determine a mass and volume relationship with an emphasis on mole concepts;
- calculate changes in enthalpy, entropy, and free energy;
- calculate reaction quotient; and
- predict the shift in reaction based on Le Chatelier's principle.

Degree of Difficulty

This problem requires students to integrate several aspects of the AP Chemistry curriculum to obtain the solution. For the average AP Chemistry student, the problem may be moderately difficult.

Class Time Required

This problem requires 40–55 minutes.

- Introduction: 5–10 minutes
  - o Read and discuss the background section with the class before students work on the problem.
- Student Work Time: 25–30 minutes
- Post Discussion:10–15 minutes

Background

This problem is part of a series of problems that apply Math and Science @ Work in NASA's research facilities.

The International Space Station (ISS) is a research laboratory assembled in low-Earth orbit. Construction of the ISS began in 1998, and it was completed in 2011. Crews aboard the ISS conduct experiments in biology, chemistry, physics, medicine, and physiology, and make observations in astronomy and meteorology. The microgravity environment of space makes the ISS a unique laboratory for the testing of spacecraft systems that will be required for future exploration missions beyond low-Earth orbit.

The ISS is operated jointly among five participating space agencies: the United States' National Aeronautics and Space Administration (NASA), the European Space Agency (ESA), the Russian Federal Space Agency (RKA),

Grade Level
11–12

Key Topic
Stoichiometry
Chemical equilibrium
Thermodynamics

Degree of Difficulty
Moderate

Teacher Prep Time
5–10 minutes

Class Time Required
40–55 minutes

Technology
Calculator

Materials
AP chemistry equation sheet

AP Course Topics
Reactions:
- Reaction Types
- Stoichiometry

NSES
Science Standards
- Unifying Concepts and Processes
- Physical Science
- Science in Personal and Social Perspectives
- History and Nature of Science

the Japan Aerospace Exploration Agency (JAXA), and the Canadian Space Agency (CSA).

Figure 1: The ISS orbiting the Earth as observed by Space Shuttle Discovery on March 7, 2011

An international crew, typically consisting of six members, resides on the ISS for approximately six months at a time. Since the first crew aboard the ISS in 1998, humans have maintained a permanent presence in space. In addition to the crews, personnel on the ground (located in Mission Control Centers) control the operations of the ISS.

Maintaining a permanent human presence on the ISS requires a well-organized and precise life support system. Flight controllers, known as Environmental and Thermal Operating Systems (ETHOS) operators, work in NASA's ISS Mission Control Center, and are responsible for the maintenance of this life support system. These operators also oversee the assembly and operation of multiple ISS subsystems and functions, including atmosphere control, supply and revitalization, internal thermal control, passive thermal control, temperature and humidity, fire detection and suppression, water recovery and management, and regenerative and emergency response. As ETHOS operators perform these duties, they are providing a safe environment for the ISS crew to live and perform valuable research in space.

AP Course Topics

Reactions

- Stoichiometry
  - Mass and volume relations with emphasis on the mole concept, including empirical formulas and limiting reactants
- Equilibrium
  - Concepts of dynamic equilibrium; physical and chemical; Le Chatelier's principle; equilibrium constants
  - Quantitative treatment
    - Equilibrium constants for gaseous reactions: K_c
- Thermodynamics
  - State Functions
  - First Law: change in enthalpy; heat of formation; heat of reaction;

- Second Law: entropy; free energy of formation; free energy of reaction; dependence of change in free energy on enthalpy and entropy changes.
- Relationship of change in free energy to equilibrium constants and electrode potentials

NSES Science Standards

Unifying Concepts and Processes

- Evidence, models, and explanation
- Change, constancy, and measurement

Physical Science

- Chemical reactions

Science in Personal and Social Perspectives

- Science and technology in local, national, and global challenges

History and Nature of Science

- Science as a human endeavor

Problem and Solution Key (One Approach)

The Sabatier Reactor is part of the Environmental Control and Life Support System (ECLSS) on the ISS. The Sabatier Reactor uses hydrogen gas and carbon dioxide to generate water and methane at a temperature of 673 K.

The hydrogen gas is obtained through water electrolysis, a function performed by another part of ECLSS (called the Oxygen Generating System). The carbon dioxide is captured from the ISS atmosphere. As a result, the water generated by the Sabatier Reactor can be purified and used as drinking water (with minerals added for taste), or can be used for other functions on the ISS. The methane is then vented into space.

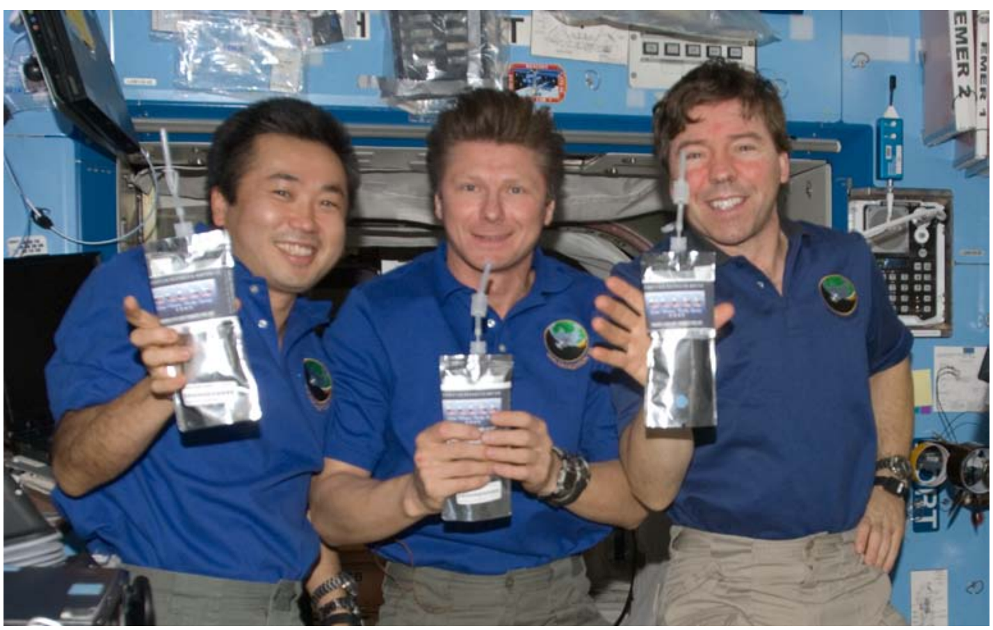

Figure 2: Expedition19 crewmembers are the first to drink recycled water produced on the ISS.

A. Using the provided information about the Sabatier Reactor and its use of hydrogen and carbon dioxide, answer the following questions in regard to the reaction.

I. Write a complete balanced equation for the equilibrium reaction between hydrogen gas and carbon dioxide.

$$4H_2(g)+CO_2(g) \rightleftharpoons 2H_2O(l)+CH_4(g)$$

II. Write the equilibrium expression, K_c, for the reaction.

$$K_c=\frac{[CH_4]}{[H_2]^4[CO_2]}$$

B. The Sabatier Reactor is projected to produce 909 kg of water per year. Calculate the number of grams of hydrogen gas that needs to be collected each month to produce this amount of water.

$$\frac{909\ kg\,H_2O}{yr}\cdot\frac{1000\ g}{1\ kg}\cdot\frac{1\,mol\,H_2O}{18.010\,g\,H_2O}\cdot\frac{4\,mol\,H_2}{2\ mol\ H_2O}\cdot\frac{2.010\,g\,H_2}{1\,mol\ H_2}\cdot\frac{1\,yr}{12\ months}=\frac{16908.1\ g\,H_2}{month}$$

$1.69\times10^4\ g\,H_2$ *need to be collected each month.*

C. Calculate the change in enthalpy, $\Delta H°_{rxn}$, for the reaction using the following bond energies.

Bond	Bond Energies (kJ per mol)
H-H	432
C=O	745
H-O	467
C-H	413

$$\Delta H°_{rxn}=4(432)+2(745)-[4(467)+4(413)]$$
$$\Delta H°_{rxn}=-3.02\times10^2\ kJ\cdot mol^{-1}\quad or\quad -3.02\times10^5\ J\cdot mol^{-1}$$

D. Calculate the change in entropy, $\Delta S°_{rxn}$, for the reaction using the following table.

Substance	ΔS° (J K^{-1} mol^{-1})
H_2	130.6
CO_2	213.6
H_2O	69.9
CH_4	186.2

$$\Delta S^\circ_{rxn} = 2(69.9) + (186.2) - \left[4(130.6) + (213.6)\right]$$
$$\Delta S^\circ_{rxn} = -4.10 \times 10^{2}\ J \cdot K^{-1} \cdot mol^{-1}\ \text{or}\ -4.10 \times 10^{-1}\ kJ \cdot K^{-1} \cdot mol^{-1}$$

E. Calculate the standard Gibbs free energy, ΔG°_{rxn}, and the Gibbs free energy, ΔG_{rxn}, at 673 K.

Standard free energy, ΔG°

$$\Delta G^\circ_{rxn} = \Delta H - T \cdot \Delta S$$
$$\Delta G^\circ_{rxn} = \left(-302\ kJ \cdot mol^{-1}\right) - (298\ K) \cdot \left(-0.410\ kJ \cdot K^{-1} \cdot mol^{-1}\right)$$
$$\Delta G^\circ_{rxn} = -1.80 \times 10^{2}\ kJ \cdot mol^{-1}\ \text{or}\ -1.80 \times 10^{5}\ J \cdot mol^{-1}$$

ΔG at 673 K

$$\Delta G_{rxn} = \Delta H - T \cdot \Delta S$$
$$\Delta G_{rxn} = \left(-302\ kJ \cdot mol^{-1}\right) - (673\ K) \cdot \left(-0.410\ kJ \cdot K^{-1} \cdot mol^{-1}\right)$$
$$\Delta G_{rxn} = -2.61 \times 10^{1}\ kJ \cdot mol^{-1}\ \text{or}\ -2.61 \times 10^{4}\ J \cdot mol^{-1}$$

F. Calculate the reaction quotient, Q, for the reaction.

$$\Delta G_{rxn} = \Delta G^\circ_{rxn} + RT\ lnQ$$
$$-26{,}100\ J \cdot mol^{-1} = \left(-180{,}000\ J \cdot mol^{-1}\right) + \left(8.314\ J \cdot K^{-1} \cdot mol^{-1}\right) \cdot (673\ K) \cdot lnQ$$
$$153{,}900\ J \cdot mol^{-1} = \left(5595.322\ J \cdot mol^{-1}\right) \cdot lnQ$$
$$lnQ = \frac{153{,}900\ J \cdot mol^{-1}}{5595.322\ J \cdot mol^{-1}}$$
$$Q = 8.82 \times 10^{11}$$

G. Based on Le Chatelier's principles and the needs of the ISS, answer the following questions.

I. Why is it critical for this process on the ISS not to reach equilibrium?

The purpose of the system is to generate water. When equilibrium is reached, the reaction shifts between products and reactants to maintain dynamic equilibrium. Therefore, water production would not occur.

II. Should the reaction quotient, Q, be less than or greater than the equilibrium constant, K? Explain your reasoning as it relates to the ISS.

Q should be less than K in order to shift reaction to the right so that more products would be made – in this case, water production.

III. With limited volume for this reaction, how would you keep the reaction flowing in the direction of the products?

By removing the methane, the Q value decreases, driving the reaction to the right and producing more water.

Scoring Guide

Suggested 11 points total to be given.

Question		Distribution of points
A	*2 points*	1 point for the correct balanced equation 1 point for the correct equilibrium expression
B	*1 point*	1 point for the correct answer
C	*1 point*	1 point for the correct $\Delta H°_{rxn}$ value
D	*1point*	1 point for the correct $\Delta S°_{rxn}$ value
E	*2 points*	1 point for the correct $\Delta G°_{rxn}$ value 1 point for the correct ΔG_{rxn} *value*
F	*1 point*	1 point for the correct reaction quotient
G	*3 points*	1 point for the correct explanation of each of the three parts

Contributors

This problem was developed by the Human Research Program Education and Outreach (HRPEO) team with the help of NASA subject matter experts and high school AP Chemistry instructors.

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